DIPPR® / AIChE® Project 991

Thermophysical Property Data Exchange

Speaker:

Ashok K. Dewan, Equilon Enterprises, LLC

DIPPR Project 991 Steering Committee Co-Chair

Dale Embry, Phillips Petroleum Company

DIPPR Project 991 Steering Committee Co-Chair

Todd J. Willman, EPCON International

DIPPR Project 991 Principal Investigator

(to whom correspondence shall be addressed)

16360 Park Ten Place, Suite 330, Houston, TX 77084, USA

e-mail: info@epcon.com

KEYWORDS

Physical Property Data Exchange, PPDX, Data Standard, Physical Properties, Model, Application

ABSTRACT

The **D**esign **I**nstitute for **P**hysical **Pr**operty Data (**DIPPR**®) under the auspices of the **A**merican **I**nstitute of **Ch**emical **E**ngineers (**AIChE**®) is developing a thermophysical property data exchange standard for DIPPR project results (e.g., DIPPR Projects 801 and 911 physical property databases). This DIPPR project – Project 991 - uses an extended version of the **I**ndustrie **K**onsortium - **C**omputer **A**ided **P**rocess **E**ngineering (**IK-CAPE**) **P**hysical **P**roperty **D**ata e**X**change (PPDX) neutral file format being developed in cooperation with the **DE**utsche Gesellschaft für **CHEM**isches **A**pparatewesen, Chemische Technik und Biotechnologie e.V (**DECHEMA**). By the end of year 2000, this thermophysical property data exchange standard will be further expanded to include other third party thermophysical property data products. Examples include the **A**merican **P**etroleum **I**nstitute (**API**) Technical Database, certain **N**ational **I**nstitute of **S**tandards and **T**echnology (**NIST**) publications, the Texas A&M University **T**hermodynamics **R**esearch **C**enter (**TRC**) Tables, and other electronic sources within and outside the USA. The developing standard is expected to be compatible with the **p**rocess **d**ata e**X**change **i**nstitute (**pdXi**) initiative under AICHE auspices. This data exchange standard will allow

any type of experimental and thermophysical property data from any of these sources to be passed to any other database, or simulation program.

INTRODUCTION

DIPPR Project 991**,** Thermophysical Property Data Exchange**,** was initiated in January of 1999 to define a standard for the exchange of thermophysical property data between DIPPR Projects (e.g. Project 801: Evaluated Process Design Data; Project 911: Environmental, Safety and Health Property Data and Estimations) and other non-DIPPR products (e.g. API Technical Database, TRC Tables, and process engineering simulators such as Aspen Plus®).

The purpose of this DIPPR sponsored project is to facilitate the easy translation of thermophysical property data among commonly used process engineering tools and the data used by process engineers to retrieve and/or calculate thermophysical property information. The driving force in defining a data exchange standard is to minimize the labor-intensive interpretation, data entry, and quality checks to insure data integrity at each transfer point. This is also anticipated to enhance the accuracy and utilization of physical property data in process engineering software by easing the use of the recommended database files from a physical property data group such as DIPPR, DECHEMA, NIST, API or TRC.

EPCON International is the principal investigator of DIPPR project 991. The project deliverables from EPCON International will include a well-defined and documented Standard - downloadable from a web site in the World Wide Web - with detailed software implementation instructions and examples to send and receive thermophysical property data to and from neutral files.

To be successful in the marketplace, a few pre-requisites are desirable:

1. Have a worldwide Standard for physical property data exchange commonly accepted by prominent groups in this arena (e.g., IK-CAPE, DECHEMA, DIPPR, AIChE, pdXi, IUCOSPED)
2. Have a test-bed of commercial products that can demonstrate the implementation and use of the standard (e.g., Aspen Technology's Aspen Plus® Process Simulator, EPCON International's interfaces for selected DIPPR and non-DIPPR physical property databases, NIST physical property databases, etc.)
3. In its current form (mid 2000), a "neutral file format" alludes to a flat ASCII file with paragraph indented keyword data structure. In the near future (end of 2000), a "neutral file format" shall define a relational database schema. The latter would allow end-users to use their own relational database tables in conjunction with the new PPDX.
4. Each data provider shall read and write its data into the standard "neutral file format". This will allow each data provider to maintain its own internal data consistency. The DIPPR 991 project will provide the necessary neutral file

format for data exchange as well as a data dictionary and examples, freely and easily downloaded from the WWW. As the Standard definition progresses, it is foreseen the publication of the Standard will be extended using meta data definition languages such as SQL and XML. In that event, the table schema and data dictionary will be published and disseminated, to allow product vendors to accept data from 3rd parties, using common relational data access tools.

There is interest to simplify the interface (or, access) to a "standardized" database neutral file format, via access from a higher level language such as the Universal Modeling Language (UML). The use of UML could facilitate the transfer of physical property data to a calling application program by defining a "CALL" statement with specified input/output arguments. This subject is beyond the scope of the current paper and will be pursued in the future, if there is sufficient user interest to do so.

5. Organize a Standing Committee that will examine extensions and modifications to keep the Data Exchange Standard evergreen. The new PPDX standard is just the **beginning** of developing and accepting a common global standard for physical property data exchange. We are looking to the other data groups and organizations to provide inputs into the PPDX standard and help to encourage and foster the use of PPDX globally. For example, with the proliferation of the World Wide Web, the XML format may provide enhanced data exchange service.

PRIOR ART

A survey by the DIPPR 991 Steering Committee of the prior art in data exchange standards already proposed, showed that the IK-CAPE-PPDX (Physical Property Data eXchange) neutral flat-file format was the best available starting point to build upon for supporting the desired interchange of physical property data. This approach of working with an existing data exchange standard was selected to avoid rework and duplication of the successful effort to date. Another advantage of this approach is that it will build momentum for this emerging standard, which was developed jointly by Aspen Technology and DECHEMA, primarily for use of DECHEMA physical property data within Aspen Plus®.

The IUCOSPED approach by Dr. Henry Kehiaian's group, supported by CODATA and IUPAC, is different. Communications with Dr Kehiaian leads us to believe that he will continue with his "SELF" format but may now plan to be consistent with the IK-CAPE/DECHEMA/DIPPR/AIChE/pdXi data exchange standard in his web based property system.

WORK in PROGRESS

During the first year (1999), the emphasis was easy translation of data between the DIPPR data compilation projects such as 801 and 911, and selected commercial process engineering software using the proposed IK-CAPE/DIPPR/AIChE/pdXi file format. This

has been demonstrated in EPCON's commercial software programs. Additionally, a subset of DIPPR 801 data was transferred from EPCON's flash program to Aspen Technology's Aspen Plus®, using the IK-CAPE PPDX neutral file format. The original IK-CAPE PPDX standard in flat-file form is now being updated in cooperation with DECHEMA and Aspen Technology who have committed to quick implementation within their software products. We have begun discussions with the Global CAPE OPEN (GCO) Project to determine how the updated version of IK-CAPE PPDX with DIPPR compatibility should be related to GCO. The DIPPR project 991 steering committee intends to submit this current neutral flat file data exchange standard to GCO for adoption. The relational file form will be ready for testing in the second half of 2000.

Project deliverable(s) for this project (anticipated at the end of 2000) will be a well-tested, documented thermophysical data exchange standard to transmit and receive thermophysical property data using the revised IK-CAPE/DIPPR/AIChE/pdXi "neutral file" format. The data exchange standard will handle property constants, temperature dependent properties, vapor-liquid and liquid-liquid mixture properties, methods used to predict data, suitable examples, implementation instructions, etc. The pdXi technical management staff has indicated support for the revised Property Data Exchange Standard within pdXi as they further tune their internal standards.

Figure 1 depicts the interactions between the various data centers on producing one proposed single global PPDX. The identified remaining changes which need to be made

to the PPDX format to accomplish wide coverage for DIPPR databases are listed in Figures 2a and 2b. An example file of PPDX using the existing set of keywords is illustrated in Figure 3. EPCON's distribution agreements with other physical property data groups including API, TRC, and the National Engineering Laboratory (NEL) will help promote dissemination of this standard.

PLANS FOR THE FUTURE

Discussions are beginning to define the interactions between DIPPR and GCO. Opportunities may exist within the GCO Work Packages to connect with DIPPR to further extend and refine PPDX, and for possible overall coordination of future improvements and refinements in this emerging global standard. Companies that desire to support further development of this new standard for interchange of physical property data are encouraged to participate in the activities of one or more of the PPDX supporting organizations: DIPPR, AIChE, IK-CAPE, DECHEMA, API, NIST, TRC, pdXi, and/or GCO.

CONCLUSION

A new single global physical property data exchange (PPDX) standard is being defined. Experimental and thermophysical property data such as the DIPPR 801 and DIPPR 911 databases, and correlations developed using statistical quality control techniques, will be directly utilized within any commercial software program, using the new PPDX standard. Rework by data specialists to reformat and rearrange thermophysical property data for

each software application will be eliminated. More attention can then be directed to the integrity of the quality control inherent in the data's original form.

The new PPDX will allow each thermophysical property data group to maintain their own proprietary data format while also providing for direct use of their data in a variety of commercial applications. The benefits of quality control and effective utilization of thermophysical property data can therefore be realized using this data exchange standard. The authors recognize that the new PPDX may not fully meet (or communicate) the needs of other constituencies (e.g., publishers, professional societies like the American Chemical Society). We expect the PPDX standard to be evergreen and evolving. As the diverse chemical community (industry, academia, publishers, etc.) profit from the use of PPDX, their concerns and needs will be folded into future editions of the PPDX standard.

ACKNOWLEDGEMENTS

We acknowledge the active participation and support of the following data groups:

1. **D**esign **I**nstitute for **P**hysical **Pr**operty Data (**DIPPR**®)
2. **A**merican **I**nstitute of **Ch**emical **E**ngineers (**AIChE**®)
3. **I**ndustrie **K**onsortium- **C**omputer **A**ided **P**rocess **E**ngineering (**IK-CAPE**)
4. **DE**utsche Gesellschaft für **CHEM**isches **A**pparatewesen, Chemische Technik und Biotechnologie e.V (**DECHEMA**)
5. **A**merican **P**etroleum **I**nstitute (**API**)
6. **N**ational **I**nstitute of **S**tandards and **T**echnology (**NIST**)

7. Texas A&M University **T**hermodynamics **R**esearch **C**enter (**TRC**)
8. **p**rocess **d**ata e**X**change **i**nstitute (**pdXi**)
9. **G**lobal **C**APE **O**PEN (**GCO**) – funded by the European Commission under the Brite-Euram program and endorsed by the Intelligent Manufacturing Systems (IMS) initiative.

Figure 1: Interactions Between Various Data Groups, Application Programs and Global PPDX

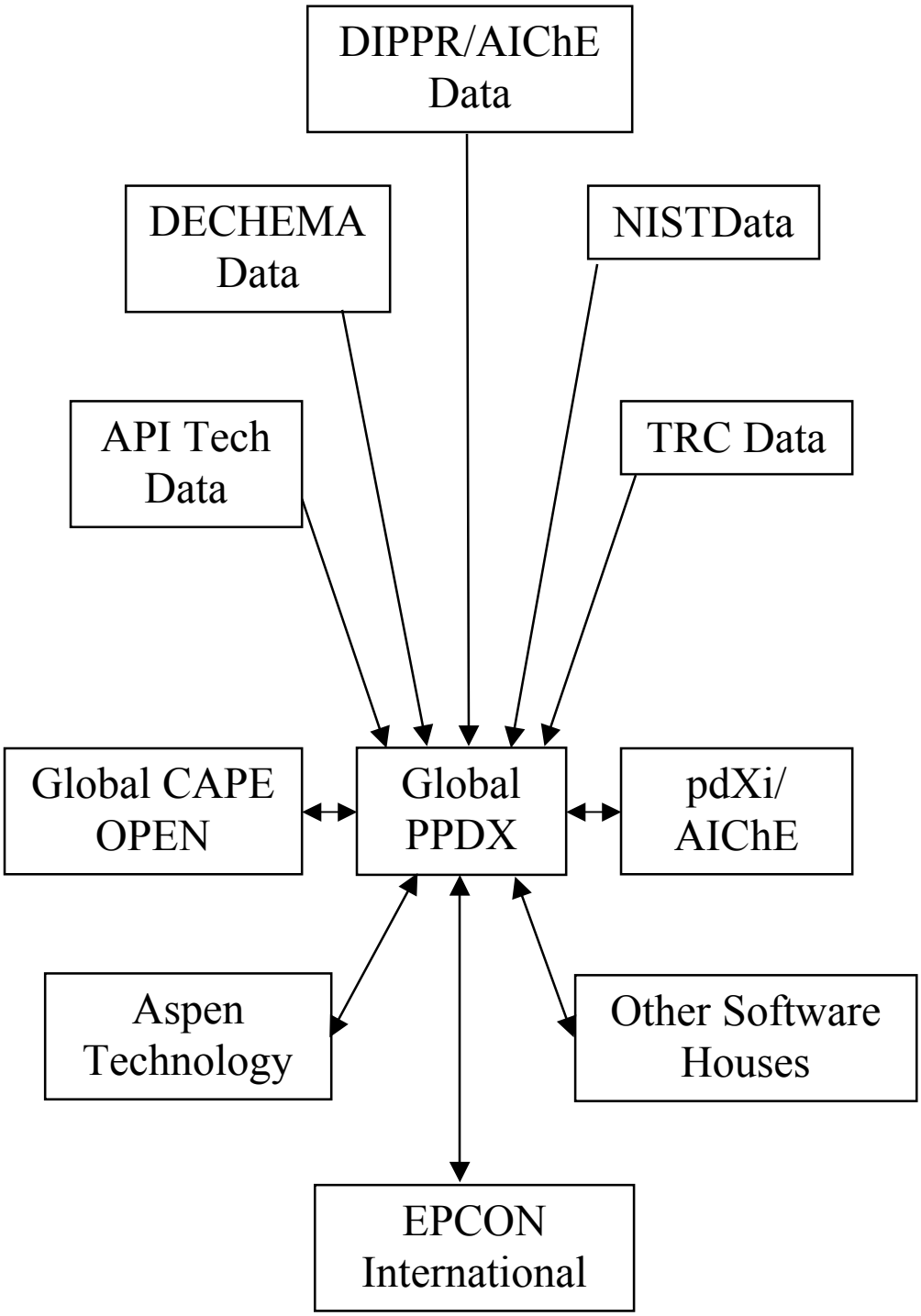

Figure 2a. Equation Forms to be Added to Revised PPDX

DIPPR_104 (Second Virial Coefficient)

$$Y = A + B/T + C/T^3 + D/T^8 + E/T^9$$

DIPPR_114 (Liquid Heat Capacity)

$$Y = \frac{A}{t} + B - 2ACt - ADt^2 - \frac{C\,t^3}{3} - \frac{CDt^4}{2} - \frac{D\,t^5}{5}$$

$$\text{where } t = (1 - T_r)$$

DIPPR_115 (Vapor Pressure)

$$\ln(Y) = A + \frac{B}{T} + C \ln(T) + DT^2 + \frac{E}{T^2}$$

DIPPR_116 (Liquid Density of Water)

$$Y = A + B(1 - T_r)^{.35} + C(1 - T_r)^{2/3} + D(1 - T_r) + E(1 - T_r)^{4/3}$$

Y = property value, T = temperature in kelvins

A, B, C, D, E = regression coefficients

Figure 2b. New Physical Properties to be Added to Revised PPDX

DIPPR 801, Evaluated Process Design Data:

Triple point temperature (TPT), K

Triple point pressure (TPP), Pa

Refractive index (RI) at 298.15 K, dimensionless

Solubility parameter (SOLP), (J/m3)^.5

van der Waals volume (VDWV), m3/kmol

van der Waals area (VDWA), m2/kmol

Flash point (FP), K

Lower flammability limit (FLML), vol% in air

Lower flammability limit temperature (FLMLT), K

Upper flammability limit (FLMU), vol% in air

Upper flammability limit temperature (FLMUT), K

Auto ignition temperature (AIT), K

Solid (or, Sublimation) Vapor Pressure (temperature dependent) (SVP), Pa

DIPPR 911, Environmental, Safety and Health Property Data and Estimations

Biological oxygen demand (BOD)

Dichromate chemical oxygen demand (COD)

Permanganate chemical oxygen demand (CODP)

Theoretical oxygen demand, carbonaceous (THOD)

Theoretical oxygen demand, carbonaceous and nitrogenous (THODN)

Octanol/water partion coefficient (KOW), dimensionless

Soil/water partion coefficient (KSW), dimensionless

Organic carbon/water partion coefficient (KOC), dimensionless

Bioconcentration factor (BCF), dimensionless

Acute aquatic toxicity, lethal concentration (LC50), species, time and sample

Acute aquatic toxicity, effective concentration (EC50), species, time and sample

Figure 3: Listing of PPDX Neutral File

```
VERSION     IKC-PPDX    1.5

PRIVATE
        KEYWORDS PRIV_KEY_1
        BLOCKS      PRIV_BLOCK_1 PRIV_BLOCK_2
END PRIVATE

QUALITY
       QKEY   1        "very good"
       QKEY   2        "good"
       QKEY   3        "average"
       QKEY   4        "bad"
END QUALITY

SOURCE
        KEY Ref-1
                AUTHOR      "Author, A.B.; Author, C.D."
                TITLE       "The title of this 'ole' document"
                JOURNAL     "A Journal"
                CODEN               JCEAAX
                VOLUME      32
                ISSUE       4
                PAGE        420-422
                YEAR        1987
                ISSN        123456789
                PRIV_KEY_1 "Mr. Meyer, Office 7.2, 7th floor"
        END KEY Ref-1
END SOURCE

COMP-DEF
        CID     MeOH
                NAME                Methanol
                FORMULA     CH4O
                SYNONYM     Holzgeist
                CAS-NO      65-12-03
                STRUCTURE JOBACK       CH3 1 OH 1
        END CID MeOH
        CID     H2O
                NAME        Water
                FORMULA     H2O
                SYNONYM     Wasser
        END CID H2O
```

```
        CID     C6H6
                NAME            Benzene
                FORMULA         C6H6
        END CID C6H6
END COMP-DEF

PURE-COMP-DATA

        PROPERTIES
                MW      $       MeOH 36.5       kg/kmol         $       $       2       Ref-1
                TB              $       MeOH 64.8    C          $       $       2       Ref-1
        END PROPERTIES

        PARAMETERS
              UNIQUAC   r       $       MeOH 3.5
              UNIQUAC   q       $       MeOH 4.1
              UNIQUAC   r       1       MeOH 3.84
              UNIQUAC   q       1       MeOH 4.67
        END PARAMETERS

        TABLE vap-press
                COMPONENT       MeOH
                SOURCE-KEY      Ref-1
                PROPERTY        PVL     T
                UNIT            mbar    C
                ERROR                   5       1
                DATA            120     10.
                DATA            180.    20.
                DATA            220     30.
                ERROR                   8.      2
                DATA            300.    50.
                DATA            1000.   4.8
        END TABLE vap-pres

        FUNCTION vap-pres
                NAME                    ANTOINE
                COMPONENT               MeOH
                QUALITY                 2
                PROPERTY                PVL     T
                UNIT                    Torr    C
                LOWER-BOUND             0.
                UPPER-BOUND             150.
                COEFFICIENTS            123.    -34.    250.
        END FUNCTION vap-pres
```

```
    PRIV_BLOCK_1
        …
        …
    END PRIV_BLOCK_1

END PURE-COMP-DATA

MIXTURE-DATA

    TABLE h
        COMPONENTS      MeOH H2O
        PROPERTY  T     X    H
        PHASE           L    L     L
        UNIT      C     mol/mol    kJ/kg
        DATA      10.   .5   2350.
        DATA      20.   .5   2360.
        DATA      10.   .6   2420.
        DATA      20.   .6   2425.
    END TABLE h

    TABLE vle
        COMPONENTS      MeOH H2O
        STATE           VLE
        PROPERTY  T     P    X     Y
        UNIT      C     bar  mol/mol     mol/mol
        DATA      60.   1.1  .5    .3
        DATA      80.   1.1  .4    .2
    END TABLE vle
```

```
TABLE lle
        COMPONENTS      H2O     MeOH C6H6
        PROPERTY  T     X       X       X       X
        PHASE           $       L1      L2      L1      L2
        UNIT      K     mol/mol         mol/mol         mol/mol
                mol/mol
        DATA      299.15 0.95886        0.00516         0.04067
                0.00798
        DATA      299.15 0.83843        0.00807         0.16052
                0.02389
        DATA      299.15 0.63984        0.01051         0.35282
                0.03783
        DATA      299.15 $      0.8383 $       0.1605
        DATA      299.15 $      0.7249 $       0.2715
        DATA      299.15 0.1218 $       0.4982 $
        DATA      299.15 0.1102 $       0.4541 $
END TABLE lle

BINARY-PARAM
        METHOD NRTL VLE Set-1
                Alpha   MeOH H2O    0.2     0.2
                A       MeOH H2O    3.5     4.3
                B       MeOH H2O    2.1     3.2
        END METHOD NRTL

        METHOD PR VLE Set-1
                K       MeOH H2O    0.12    0.12
                K       MeOH C6H6   0.02    0.02
                K       H2O  C6H6   0.21    0.21
        END METHOD PR

        METHOD PR VLE Set-EOS
                K       MeOH H2O    0.11    0.11
                K       MeOH C6H6   0.82    0.82
                K       H2O  C6H6   0.23    0.23
        END METHOD PR

        METHOD NRTL LLE Set-1
                Alpha   MeOH H2O    0.3     0.3
                A       MeOH H2O    1.1     2.2
                BOUNDS-T    0       100     C
                BOUNDS-X    0       0.2     mol/mol     L1      MeOH
                BOUNDS-X    0.9     1.0     mol/mol     L2      MeOH
        END METHOD NRTL
```

```
        END BINARY-PARAM

        PRIV_BLOCK_2
                …
                …
        END PRIV_BLOCK_2

END MIXTURE-DATA

GROUP-METHODS

        G-PARAMETER
                METHOD D-UNIF    r       q
                        CH3     1       2.5     3.8
                        OH      5       1.2     2.7
                END METHOD D-UNIF
        END G-PARAMETER

        G-INTERACTION
                METHOD D-UNIF
                        B       1       3       1.1     2.3
                        B       1       5       2.0     1.1
                        B       5       7       2.3     2.2
                END METHOD D-UNIF
        END G-INTERACTION

END GROUP-METHODS

THERMODYNAMIC T1
        VLEQ
                ACTIVITY    NRTL  Set-1
                FUGACITY    PR    Set-1
                POYNTING    TRUE
        END VLEQ

        LLEQ
                ACTIVITY    NRTL  Set-1
        END LLEQ

        ENTHALPY
                ACTIVITY    NRTL  Set-1
                PRESS-CORR  PR    Set-1
                STARTPHASE        MeOH L
                STARTPHASE        H20  L
```

```
            STARTPHASE      C6H6  V
            TREF            H20   298.15 K
            TREF            MeOH  298.15 K
            TREF            C6H6  298.15 K
            HREF            H2O   23.000 J/mol
            HREF            MeOH  12.230 J/mol
            HREF            C6H6  45.560 J/mol
            T-PH-CH         H2O   340    K
            T-PH-CH         MeOH  340    K
            T-PH-CH         C6H6  323.15 K
        END ENTHALPY

        MIXCALC
            VIS    L        MOLA
            DENS   V        PR    Set-1
        END MIXCALC
END THERMODYNAMIC T1

THERMODYNAMIC T2
        BASIC T1
        VLEQ
            EOS             PR    SET-EOS
        END VLEQ
END THERMODYNAMIC T2

SYSTEM S1
        COMPONENTS          MeOH H2O
        THERMODYNAMIC T1
END SYSTEM S1

SYSTEM S2
        COMPONENTS          MeOH H2O   C6H6
        THERMODYNAMIC T2
END SYSTEM S2
```